Pseudogaps due to sound modes: from incommensurate charge density waves to semiconducting wires.

S. A. Brazovskii[1,2] and S.I. Matveenko[2,1]

[1]*Laboratoire de Physique Théorique et des Modèle Statistiques,*
CNRS, Bât.100, Université Paris-Sud, 91405 Orsay cedex, France.
[2]*L.D. Landau Institute for Theoretical Physics,*
Kosygina Str. 2, 117940, Moscow, Russia.
(06/08/02)

Abstract

We consider pseudogap effects for electrons interacting with gapless modes. We study both generic 1D semiconductors with acoustic phonons and incommensurate charge density waves. We calculate the subgap absorption as it can be observed by means of the photo electron or tunneling spectroscopy. Within the formalism of functional integration and the adiabatic approximation, the probabilities are described by nonlinear configurations of an instanton type. Particularities of both cases are determined by the topological nature of stationary excited states (acoustic polarons or amplitude solitons) and by presence of gapless phonons which change the usual dynamics to the regime of the quantum dissipation. Below the free particle edge the pseudogap starts with the exponential (stretched exponential for gapful phonons) decrease of transition rates. Deeply within the pseudogap they are dominated by a power law, in contrast with nearly exponential law for gapful modes.

PACS numbers: 72.15.Nj 78.40.Me 78.70.Dm 71.45.Lr

I. INTRODUCTION: PSEUDOGAPS IN 1D.

This article is devoted to theory of pseudogaps (PGs) in electronic spectras in applications to Photo Electron Spectroscopy (PES). We shall study an influence of quantum lattice fluctuations upon electronic transitions in the subgap region for one-dimensional ($1D$) systems with gapless phonons. Low symmetry systems with gapful spectra have been addressed by the authors recently [1] and we refer to this article for a more comprehensive review and references. Here we will show that sound branches of phonon spectra change drastically the transition rates making them much more pronounced deeply within the PG. We shall consider two types of systems: generic $1D$ semiconductors with acoustic e-ph coupling (conducting polymers, quantum wires, nanotubes) and Incommensurate Charge Density Waves (ICDWs) [2] which possess the gapless collective phase mode.

The PG concept [3] refers to various systems where a gap in their bare electronic spectra is partly filled showing subgap tails. Even for pure systems and at temperature $T = 0$ there may be a rather smeared edge E_g^0 while the spectrum extends deeply inwards the gap till some absolute edge E_g which may be even zero (no true gap at all). A most general reason is that stationary excitations (eigenstates of the total electron-phonon $e - ph$ system) are the self-trapped states, *polarons* or *solitons*, which energies, W_p or W_s, are below the ones of free electrons thus forming the absolute edge at $E_g < E_g^0$. Nonstationary states filling the PG range $E_g^0 > E > E_g$ can be observed *only via instantaneous measurements* like optics, PES or tunneling. Particularly near E_g^0 the states resemble free electrons in the field of *uncorrelated quantum fluctuations* of the lattice [4]; here the self-trapping has not enough time to be developed. But approaching the exact threshold E_g, the excitations evolve towards eigenstates which are *self-trapped $e - ph$* complexes. The PGs must be common in $1D$ semiconductors just because of favorable conditions for the self-trapping [5]. Further on, the PG is especially pronounced when the bare gap is opened spontaneously as a symmetry breaking effect. In quasi-$1D$ conductors it is known as the Peierls-Fröhlich instability leading to the CDW formation. Here the picture of the PG has been suggested first theoretically [3] (recall also [6] and another model [7]) in relation to absence of the long range order in $1D$ CDWs at finite temperature. In this approach the smearing of the mean field electronic gap $2\Delta_0$ corresponds to disappearance of the true Peierls-Fröhlich transition in favor of a smooth crossover. The PG shape was related, and derived from, the temperature dependent finite correlation length ξ. An alternative picture was suggested in [4] and further developed in [8]. It concentrates on effects persistent even at zero temperature which are due to strong interaction between bare electronic excitations and perturbations (amplitude and phase phonons) of the CDW ground state. Here the PG in instantaneous electronic spectra becomes related to transformation of electrons into solitons.

Experimentally, the PGs in ICDWs were addressed first by optic [9–11] and more recently by the PES and ARPES [12]. The theoretical interpretation of earlier experiments was done in [13] by compilation of approaches from [3,4,7]. Detailed theories of the subgap absorption in optics have been developed already for systems with low symmetries (nondegenerate, like semiconductors with gapful phonons, or discretely degenerate like the dimerized Peierls state). They addressed first a general type of polaronic semiconductors [14] with emphasis to long range Coulomb effects, and the $1D$ Peierls system emphasizing solitonic processes [15]. Recently the authors [1] extended the theory of pseudogaps to single electronic spectra

in application to the PES and, particularly intriguing, to the ARPES (momentum resolved PES) probes. But properties of ICDWs are further complicated by appearance of the gapless collective mode which bring drastic changes. The case of acoustic polarons (APs) in a 1D semiconductor belongs to the same class while it is not usually noticed.

Specifics of $1D$ systems with continuous degeneracy (with respect to the phase for the ICDW, to displacements for usual crystals) is that even single electronic processes can create topologically nontrivial excitations, the solitons. Thus for the ICDW a single electron or hole with energy near the gap edges $\pm\Delta_0$ spontaneously evolve to the nearly amplitude soliton - AS whilst the original particle is trapped at the local level near the gap center. The energy $\approx 0.3\Delta_0$ is released, at first sight within a time $\omega_{ph}^{-1} \sim 10^{-12}s$. We will see that actually there is also a long scale adaptation process which determines shapes of transition probabilities. Similarly, the usual acoustic polaron in a 1D semiconductors is characterized by the electronic density ρ selflocalized within the potential well $\sim \partial\varphi/\partial x \sim \rho$, hence a finite increment $\varphi(+\infty) - \varphi(-\infty) \sim \int \rho dx$ of the lattice displacements φ over the length x which is the signature of topologically nontrivial solitons. These systems with continuous degeneracy form a special class which shows particular properties and must be studied differently than in [1]. They are addressed in this article.

II. FUNCTIONAL INTEGRALS AND INSTANTONS FOR THE PES.

The absorption rate $I(\Omega, P)$, as a function of frequency (Ω and momentum P, for the ARPES can be expressed in terms of the spectral density of the one-electron retarded Green function $G(t, t'; x, x')$ as

$$I(P, \Omega) \propto Im \int dX e^{-iPX} \int_0^\infty dT e^{i\Omega T} G(X, T, 0, 0). \qquad (1)$$

We shall address here the simple PES, non resolved in momenta, measures the integrated absorption intensity $I(\Omega) = \int I(P, \Omega) dP / 2\pi$. (Since now on we shall omit all constant factors and take the Plank constant $\hbar = 1$; Ω will be measured with respect to a convenient level: the band edge for semiconductors or the middle of the gap for CDWs.)

We shall use the adiabatic approximation valid when changes of electronic energies are much larger than relevant phonon frequencies. Electrons are moving in the slowly varying phonon potential, e.g. $Re\{\Delta(x, t) \exp[i2k_F x]\}$ for the ICDW, so that at any instance t their energies $E(t)$ and wave functions $\psi(x, t)$ are defined as eigenstates for the instantaneous lattice configuration and they depend on time only parametrically. In the following we shall work in the Euclidean space $it \rightarrow t$ which is adequate for studies of classically forbidden processes [14,16,17]. Then in the form of functional integrals over lattice configurations we have

$$I(\Omega) \propto \int_0^\infty dT \int D[\Delta(x, t)] \psi_0(0, T) \psi_0^+(0, 0) e^{-S}, \qquad (2)$$

Here ψ_0 is the wave function of the particle (for the PES it is actually a hole) added and extracted at moments 0 and T. For calculations of subgap processes only the lowest singly filled localized state is relevant which energy E_0 is split off inside the gap. The action

3

$$S = S[\Delta(x,t), T]$$

$$S = (\int_{-\infty}^{0} + \int_{T}^{\infty})dt\, L_0 + \int_{0}^{T} dt\,(L_1 - \Omega),\ L_1 - L_0 = E_0 \tag{3}$$

is given by Lagrangians $L_j[\Delta]$ where the labels $j = 0, 1$ correspond to ground states for $2M$ (the bare number) and $2M \pm 1$ electrons in the potential $\Delta(x,t)$. The main contribution comes from saddle points of S, the instantons, which are extremas with respect to both the function $\Delta(x,t)$ and the time T. There are also special cases [1], particularly important for the ARPES, when the extremum must be taken for the whole expression in the integral (2), taking into account the wave functions in the prefactor. Otherwise we obtain for the stationary point $dS/dT = 0$, that is $E_0(0) = E_0(T) = \Omega$ which determines $T(\Omega)$.

In the following we shall concentrate on most principle features leaving aside calculations of prefactors and the question of the momentum dependence necessary for the ARPES. For a simpler case of nondegenerate systems they have been studied in [1].

III. CREATION OF AMPLITUDE SOLITONS IN ICDWS.

Consider first the subgap electronic spectra for the ICDW described by the Peierls-Fröhlich model. The ICDW order parameter is the complex field $\Delta = |\Delta(x,t)| \exp[i\varphi(x,t)]$ acting upon electrons by mixing states near the Fermi momenta points $\pm k_F$. The Lagrangians L_j consist of the bare kinetic $\sim |\partial_t \Delta|^2$ and potential $\sim |\Delta|^2$ lattice energies and of the sum over the filled electron levels, in the j-th state:

$$L_j = \int dx\, 2|\partial_t \Delta|^2/(\pi v_F \omega_0^2) + V_j[\Delta(x,t)]$$

where v_F is the Fermi velocity in the metallic state and $\omega 0$ is the amplitude mode frequency. ($\omega_0 \ll \Delta_0$ is the condition for the adiabatic approximation.)

The important fact is that the stationary state of the system with an odd number of particles, the minimum of V_1, is the amplitude soliton (AS) $\Delta \Rightarrow -\Delta$ with the midgap state $E_0 = 0$ occupied by the singe electron. Evolution of the free electron with the initial $E_0 = \Delta_0$ to the AS with $W_s = 2/\pi\Delta_0 < \Delta_0$ can be fortunately described by the known exact solution for intermediate configurations characterized by the single intragap $E_0 = \Delta_0 \cos\theta$ with $0 \le \theta \le \pi$, hence $-\Delta_0 \le E_0 \le \Delta_0$. It was found [8], see also reviews [18,19], to be the Chordus Soliton (ChS) with 2θ as the total chiral angle: $\Delta(+\infty)/\Delta(-\infty) = \exp(2i\theta)$, see Fig.1 and the Appendix for details. The filling number of the intragap state $\nu = 0, 1$ corresponds to labels $j = 0, 1$. The term $V_0(\theta)$ increases monotonically from $V_0(0) = 0$ for the $2M$ GS to $V_0(\pi) = 2\Delta_0$ for the $2M + 2$ GS with two free holes. The term $V_1(\theta) = V_1(\pi - \theta)$ is symmetric describing both the particle upon the $2M$ GS and the hole upon the $2M + 2$ GS. Apparently $V_1(0) = V_1(\pi) = \Delta_0$ while the minimum is reached at $\theta = \pi/2$ that is for the purely AS: $\min V(\theta) = V_1(\pi/2) = W_s < \Delta_0$ where $W_s = 2\Delta_0/\pi$ is the AS energy, see Fig.2. Thus, to create a nearly AS with $\theta = 90°$, the light with $\Omega \approx W_s$ is absorbed by the quantum fluctuation with $E_0(\theta) = W_s$ which is close to the chordus soliton with the angle $\theta \approx 50°$.

Notice that being the uncharged spin carrier with the topological charge equal unity, the AS is a quasiclassical realization of the *spinon* in systems with nonretarded attraction

of electrons (that is with high, rather than low, phonon frequencies). Thus our analysis is applied qualitatively also to arbitrary nonadiabatic electronic systems provided that they are found in the spin gap regime. (See also the next chapter.)

Usually it is tempting to use the static solution, with some free parameter, as an Anzatz for the time dependent process which proved to be successful in gapful cases [1,15]. But here, putting $\theta \to \theta(t)$, we would arrive at $\partial_t \Delta \neq 0$ at all x hence the action would be infinite $S \sim$ *the system length*. The vanishing probability simply reflects the fact that a globally finite perturbation, characteristic for topologically nontrivial solitons, cannot spread over the whole length by a finite time. More generally, as a topologically nontrivial object, the AS cannot be created in a pure form: adaptational deformations must appear to compensate for the topological charge. These deformations are developing over long space-time scales which can be described in terms of the gapless mode, the phase φ, alone. Hence allowing for the time evolution of the chiral angle $\theta \to \theta(t)$ within the core, we should also unhinder the field $\varphi \to \varphi(x,t)$ at al x and t. The resulting trajectory is shown at the Fig.1 for an instant of time. Starting from $x \to -\infty$ and returning to $x \to \infty$ the configuration follows closely the circle $|\Delta| = \Delta_0$ changing almost entirely by phase. Approaching the soliton core the phase matches approximately the angles $\pm \theta$ which delimit the chordus part of the trajectory. The whole trajectory is closed which allows for the finite action.

Except for a short time scale $T < \xi_0/u$ (see Ch.IV C) characterized by small θ and large lengths $\xi = \xi_0/\sin\theta$, the configuration $\Delta(x,t)$ can be divided into the inner part, the core at $|x| \sim \xi$, and the outer part $|x| \gg \xi$ where only perturbations of the phase $\varphi(x,t)$ are important. The inner part can be described by the chordus soliton $\Delta_{ChS}(x,t)$. The chordus angle $2\theta(t)$ evolves in time from $\theta(\pm\infty) = 0$ to θ_m in the middle of the T interval. For $T \to \infty$, that is near the stationary state of the AS, $\theta_m \to \pi/2$. Actually this value is preserved during most of the T interval so that changes between $\theta = 0$ and $\theta = \pi/2$ are concentrated within finite ranges $\tau_0 \sim \xi_0/u \ll T$ near the termination points. From large scales we view only a jump $\varphi(x,t) \approx \theta(t)\mathrm{sgn}(x)$ with $\theta(t) \approx \theta_m\Theta(t)\Theta(T-t)$ (Θ is the standard step function). Since the configuration stays close to the AS during the time T, the main core contribution to the action is

$$S_{core} = (W_s - \Omega)T + \delta S_{core} \qquad (4)$$

where the first correction $\delta S^0_{core} = cnst$ comes form regions around moments $0, T$ independently. The significant T dependent contribution $\delta S(T)$ comes from interference of regions 0 and T. Their interaction via gapful excitations like the amplitude mode decays exponentially as $\delta S_{gap} \sim \exp(-\omega_0 T)$ and for low symmetry systems there was no other contribution. But now, for the ICDW, there are *sound modes providing the main effect* which is addressed below.

Matching the inner and outer regions is not well defined unless we consider a full microscopic time dependent model which is not possible. But fortunately the long range effects can be treated easily if we generalize the scheme suggested earlier for static problems of solitons at presence of interchain interactions [20,8]. The outer region is described by the action for the sound like phase mode

$$S_{snd}[\varphi(x,t), \theta(t)] = \frac{v_F}{4\pi} \int \int dx dt \left((\partial_t \varphi/u)^2 + (\partial_x \varphi)^2 \right) , \quad \varphi(t, x_s \pm 0) = \mp\theta(t) \qquad (5)$$

where u is the phase velocity. The action S_{snd} takes into account the source provided by the chordus soliton forming around x_s which enforces the discontinuity of 2θ. Integrating out $\varphi(x,t)$ from $\exp\{-S_{snd}[\varphi,\theta]\}$ with this condition we arrive at the action for $\theta(t)$

$$S_{snd}[\theta] \approx \frac{v_F/u}{2\pi^2} \int\int dt_{1,2} \dot{\theta}(t_1) \ln|(t_1-t_2)|\dot{\theta}(t_2) = \frac{v_F/u}{2\pi^2} \int\int dt_{1,2} \left(\frac{\theta(t_1)-\theta(t_2)}{t_1-t_2}\right)^2 \tag{6}$$

Here the last form is a typical action for the problem of quantum dissipation [21] $S \sim \sum |\omega||\theta_\omega|^2$. In our case this dissipation comes from emission of phase phonons while forming the long range tail in the course of the chordus soliton development. This action, together with V_j, can be used to prove the above statements on the time evolution of the ChS core.

Remember now that $\dot{\theta} = \partial_t \theta$ is peaked within narrow regions $\sim \xi_0/u$ around moments $t=0$ and $T=0$ and close to zero otherwise. Then

$$S_{snd} \approx (v_F/4u)\ln(uT/\xi_0) \tag{7}$$

There is an even more phenomenological point of view, see [22] on more details and examples for combined topological defects. The AS creates the $\pi-$ discontinuity along its world line $(0 < t < T, 0)$. To be topologically allowed, that is to have a finite action, the line must terminate with half integer vortices located at $(0,0)$ and $(0,T)$ which circulation will provide the compensating jump $\delta\varphi = \pi$ along the interval ($\Delta \Rightarrow -\Delta$ combined with $\varphi \Rightarrow \varphi + \pi$ leaves the order parameter $\Delta\exp(i\varphi)$ invariant). Then the standard energy of vortices for (5) leads to the action (7). Contrary to usual $2\pi-$ vortices, the line connecting the half-integer ones is the physical singularity which tension gives (4).

Minimizing $S_{tot} = S_{core} + S_{snd}$ with respect to T, we obtain near the AS edge $\Omega \geq W_s$ the power law

$$I(\Omega) \propto \left(\frac{\Omega - W_s}{W_s}\right)^\beta , \quad \beta = \frac{v_F}{4u} \tag{8}$$

which is much more pronounced than the exponential law (see (15) below) for gapful cases.

Our derivation suggests literally the long range order at large (x,t) distances and neglects fluctuations of the phase except perturbations enforced by the instanton. But the mean fluctuations of the phase diverge and the order parameter decays in a power law. These long range fluctuations are not related to the instanton and can be taken into account *a posteriori*. (Actually we have been using only the discontinuity condition leaving the phase free at infinity.)It is easy to do by noticing that the eigenfunctions in the prefactor of (2) transform as $\Psi_0 \Rightarrow \Psi_0 \exp\{i/2\,\varphi(x,t)\}$ which averaging contributes the action term

$$\delta S_\varphi = 1/8 < [\varphi(0,0) - \varphi(0,T)]^2 > \approx (u/4v_F)\ln(uT/\xi_0) .$$

Thus the effect of phase fluctuations, as well as the major role of the form Factor, is simply to correct the value of the index in (8) as $\beta \Rightarrow \beta^* = v_F/4u + u/4v_F$. Within our adiabatic approximation $u/v_F \ll 1$ the correction is small but it builds a bridge to quantum nonadiabatic models where exactly the combination of β^* appears as the index of the single particle Green function with $\gamma_\rho = u/v_F$ being identified as the charge channel exponent.

The link is completed by noticing that the AS is a realization of the spinon and that the phase discontinuity in (5) is equivalent, together with fluctuations, to applying the operator

$$\exp\left\{\frac{i}{2}\varphi(x,t) + i\frac{\pi}{2}\frac{\delta}{\delta\varphi}\mathrm{sgn}x\Theta(t)\Theta(T-t)\right\}$$

which is our limit for the bosonization.

IV. ACOUSTIC POLARON AND THE FREE EDGE.

A. 1D semiconductors with acoustic and optical polarons.

Behavior near the free edge $\Omega \approx \Delta_0$ is dominated by small fluctuations η of the gap amplitude $|\Delta| = \Delta_0 + \eta$ and of the Fermi level $\delta E_F = \varphi' v_F/2$ via the phase gradient $\varphi' = \partial_x\varphi$. We shall consider it in a frame of a generic problem of the combined (gapful and acoustic) polaron. The more simple, in compare to the CDW, single particle formulation bares similar qualitative features but allows for a more detailed analysis. Consider electron (hole) states in a 1D dielectric near the edge of a conducting (valence) band. We shall take into account the gapful mode η with the coupling g_0 and the sound mode (for which we shall keep the "phase" notation φ) with the velocity u and the coupling g_s. In generic semiconductors the sound mode is always present as the usual acoustic phonon while the gapful mode can be present as an additional degree of freedom. In all CDWs the gapful mode is always present as the amplitude fluctuation $|\Delta| = \Delta_0 + \eta$ while the sound mode appears in the ICDWs as the phase $\Delta = |\Delta|\exp[i\varphi]$.

Within the adiabatic approximation for the electron's wave function Ψ the action S (at the imaginary time) has the form

$$S = \int dx \int_0^T dt \left[\left(\frac{1}{2m}|\partial_x\Psi|^2 - \Omega|\Psi|^2\right) + (g_s\partial_x\varphi + g_0\eta)\Psi^\dagger\Psi\right] +$$
$$\int dx \int_{-\infty}^\infty dt \left[\frac{K_s}{2}\left((\partial_t\varphi/u)^2 + (\partial_x\varphi)^2\right) + \frac{K_0}{2}\left((\partial_t\eta/\omega_0)^2 + \eta^2\right)\right]. \tag{9}$$

Thus for the ICDW case we have $m = \Delta_0/v_F^2$, $g_0 = 1$, $g_s = v_F/2$, $K_s = v_F/2\pi$, $K_0 = 4/\pi v_F$, $2^{3/2}u/v_F = \omega_0/\Delta_0$ and Ω is counted with respect to the edge Δ_0 rather than to the middle of the gap is in the previous chapter.

It is well known [5] that the stationary state, the time independent extremum of (9), corresponds to the selftrapped complex, the polaron. Here it is composed equally by both η and φ' which contribute additively to the static coupling (while the dynamics will be completely different)

$$\lambda = \lambda_s + \lambda_0 = \frac{g_s^2}{K_s} + \frac{g_0^2}{K_0}$$

The polaronic length scale l for $\eta \sim \varphi' \sim |\Psi|^2 \equiv \rho_p(x)$ is $l = 2/m\lambda$ and the total energy is $W_p = -m\lambda^2/24$. The conditions $|W_p| \gg \omega_0$ and $\lambda \gg u$ define the adiabatic, Born - Oppenheimer, approximation. For the CDW case $\lambda_s = v_F\pi/2$ and $\lambda_0 = v_F\pi/4$ hence $\lambda \sim v_F$ and we would arrive at $|W_p| \sim \Delta_0$ and $l \sim \xi_0 = v_F/\Delta_0$ which are the microscopic

scales where the single electronic model may be used only qualitatively. The full scale approach for nearly stationary states has been considered above in Ch.III, but the upper PG region near the free edge Δ_0 will be described by the model (9) even quantitatively and most efficiently.

We can integrate out the fields φ and η at all (x,t) to obtain the action in terms of ψ alone which is defined now only at the interval $(0,T)$ for t:

$$S\{\Psi;T\} = \int dxdt \left(\frac{1}{2m} |\partial_x \Psi|^2 - \Omega |\Psi|^2 \right) - \frac{1}{2} \int \int dt_{1,2} \int \int dx_{1,2}$$
$$\{U_0(x_1 - x_2, t_1 - t_2)\rho(x_1,t_1)\rho(x_2,t_2) + U_s(x_1 - x_2, t_1 - t_2)\partial_x\rho(x_1,t_1)\partial_x\rho(x_2,t_2)\} \qquad (10)$$

Here the self-attraction retarded potentials are

$$U_s = \frac{\lambda_s u}{2\pi} \ln \sqrt{x^2 + t^2 u^2}\,, \ U_0 = \frac{1}{2}\lambda_0\omega_0 \exp[-\omega_0|t|]\delta(x) \qquad (11)$$

An equivalent form, suitable at large T, is obtained via integrating by parts

$$S\{\Psi;T\} = \int dx \int_0^T dt \left[\frac{1}{2m} |\partial_x \Psi|^2 - \Omega\rho - \frac{\lambda}{2}\rho^2 \right] +$$
$$\frac{1}{2} \int \int dt_{1,2} \int \int dx_{1,2}\partial_t\rho(x_1,t_1)\partial_t\rho(x_2,t_1)U(x_1 - x_2, t_1 - t_2) \qquad (12)$$

where $U(x,t) = u^{-2}U_s + \omega_0^{-2}U_0$.

The absorption near the absolute edge $\Omega \approx W_p$ is determined by the long time processes when the lattice configuration is almost statically self-consistent with electrons. The first term in (12) is nothing but the action S_{st} of the static polaron which extremum at given T is

$$S_{st} \approx -T\delta\Omega\,, \ \delta\Omega = \Omega - W_p\,.$$

The second term in (12) S_{tr} collects contributions only from short transient processes near the impact moments $t = 0, T$ which are seen by the long length part as $\partial_t\rho(x,t) \approx \rho_p(x)[\delta(t) - \delta(t - T)]$ where ρ_p is the density for the static polaron solution. We obtain

$$S_{tr} \approx \int \int dx_{1,2}\rho_p(x_1)\rho_p(x_2)U(x_1 - x_2, T)$$
$$= \frac{\lambda_s}{2\pi u} \ln \frac{uT}{l} + C_0\frac{\lambda_0/l}{\omega_0} \exp[-\omega_0 T] + cnst$$

with $C_0 \sim 1$. We see the dominant contribution of the sound mode which grows logarithmically in T while the part of the gapful mode decays exponentially. If the sound mode is present at all, then the extremum over T is

$$T \approx \frac{\lambda_s}{2\pi u}\frac{1}{\delta\Omega}\,, \ S \approx \frac{\lambda_s}{2\pi u} \ln \frac{C_s|W_p|}{\delta\Omega}\,, \ C_s \approx 0.9 \qquad (13)$$

We find that near the absolute edge $\Omega \approx W_p$ the absorption is dominated by the power law with an index α which must be big within our adiabatic assumption $\alpha \gg 1$:

$$I \sim \left(\frac{\delta\Omega}{|W_p|} \right)^\alpha\,, \ \alpha = \frac{\lambda_s}{2\pi u} \qquad (14)$$

8

For parameters of the ICDW we obtain $\alpha = v_F/4u$ in full accordance with the exact treatment (8).

Only in absence of sound modes $\lambda_s = 0$ the gapful contribution can determine the absolute edge. Then the minimization over T of $S = S_{core} + \delta S_{gap}$ would lead qualitatively to the result of [1]:

$$T \sim \omega_0^{-1} \ln \left| \frac{W_p}{(W_p - \Omega)} \right| \ , \ I \sim \exp \left(-cnst \frac{|W_p|}{\omega_0} + \frac{\Omega - W_p}{\omega_0} \ln \left| \frac{W_p}{(\Omega - W_p)} \right| \right) \tag{15}$$

for $\Omega \approx W_p$.

B. Free edge vicinity.

Consider the opposite regime near the free edge $\Omega \approx 0$ ($\Omega \Rightarrow \Omega - \Delta_0$ for the ICDW). Here, entering the PG at $\Omega < 0$, the absorption is determined by fast processes of quantum fluctuations: their characteristic time $T = T(\Omega)$ is short in compare to the relevant phonon frequency: $T \ll \omega_0, u/L$, where $L = L(\Omega)$ is the characteristic localization length for the fluctuational electronic level at $E_0 = \Omega$. Since T is small, we can neglect all variations in time within $(0, T)$. Then we estimate the action (10), term by term, as

$$S \approx \frac{C_1 T}{mL^2} - \Omega T - C_2 \lambda_s u \left(\frac{T}{L} \right)^2 - C_3 \lambda_0 \omega_0 \frac{T^2}{L} \tag{16}$$

with $C_i \sim 1$. Its extremum over both L and T yields

$$S \sim \frac{|\Omega|^{3/2}/m^{1/2}}{\max \left\{ |m\Omega|^{1/2} u \lambda_s; \omega_0 \lambda_0 \right\}}$$

which provides a reasonable interpolation for the absorption in the closest and the more distant vicinities of the free electronic edge. For the purely acoustic case $\lambda_0 = 0$, a variational estimation for the numerical coefficient as $C_1 \approx 1/6, C_2 \approx 0.06$ gives

$$I \sim \exp[-cnst|\Omega|/mu\lambda_s] , \ cnst \approx 2.8 \tag{17}$$

The validity condition $uT/L \sim \sqrt{-\Omega/W_p} \ll 1$ is satisfied by definition of the edge region. This condition is compatible with the low boundary for the frequency: $S \gg 1$ hence $-\Omega/W_p \gg u/\lambda_s$, which is small as our basic adiabatic parameter.

For gapful phonons alone, $\lambda_s = 0$, we arrive at the known result (see [1] and references therein) $I \sim \exp[-cnst|\Omega|^{3/2}/\omega_0]$, $\Omega < 0$. But it was not quite predictable that among the laws $S \sim |\Omega|^{3/2}$ and $S \sim |\Omega|$ this is the smallest contribution to S which wins: $\sim |\Omega|^{3/2}$ at lowest $|\Omega|$ and $\sim |\Omega|$ for larger $|\Omega|$. For the ICDW particularly, we have $\lambda_0/\lambda_s \sim 1$ and $u/\omega_0 \sim \xi_0$, then there is no space for the intermediate asymptotics $\ln I \sim \Omega$ at $|\Omega| \ll \Delta_0$: beyond the region with $S \sim |\Omega|^{3/2}$ dominated be the amplitude fluctuations, the phase-only description is not valid and the particular nature of amplitude solitons must be taken into account. This regime has been considered above in Ch.III.

9

Actually the difference between the laws $\log I \sim -|\Omega|/u$ and $\log I \sim -|\Omega|^{3/2}/\omega_0$ can be easily interpreted. Indeed, for gapful phonons we expect the frequency scale to be $\omega_0 \Rightarrow \omega_k = uk \sim u/L \sim u|\Omega|^{1/2}$ where $k \sim 1/L$ is a characteristic wave number and L is the localization length of the fluctuation providing the bound state at $-\Omega$. Then $|\Omega|^{3/2}/\omega_0 \Rightarrow |\Omega|^{3/2}/\omega_k \sim |\Omega|/u$.

While the law (17) looks to be the simplest one, actually it is quite uncommon and its derivation is problematic in all systems, cf. [14]. In our case we notice that only at $\lambda_0 \neq 0$ the action (16) has a usual saddle point: minimum over L and maximum over T. But for the purely acoustic case $\lambda_0 = 0$ the minimum over L appears only along the extremal line over T. Contrarily, at a given T the action collapses to either $L \to 0$ or to $L \to \infty$ depending on a value of T with respect to the threshold $T^* \sim (mu\lambda_s)^{-1}$ which is just the inverse width in (17). The paradox can be resolved inspecting the generic real time formulation (2). But a necessary insight will be obtained more easily by another treatment presented in the next section.

C. Quantum fluctuations as an instantaneous disorder with long rang space correlations.

It has been noticed already that in a one dimensional system the optical absorption near the band edge can be viewed as if for a quenched disorder which is emulated by instantaneous quantum fluctuations. This asymptotically exact reduction to the time independent model can be done as follows. After neglecting the retardation at $T \ll \omega_0, u/L$, the self-interaction term in (10) can be decoupled back by the Hubbard-Stratonovich transformation via the *time independent* field ζ with the correlator $D(x) = U_0(x,0) + \partial_x^2 U_s(x,0)$:

$$S\{\Psi, \zeta; T\} = T \int dx \left(\frac{1}{2m} |\partial_x \Psi|^2 + \zeta(x)\rho(x) \right) + \frac{1}{2} \int \int dx_{1,2} \zeta(x_1) D^{-1}(x_1 - x_2) \zeta(x_2) \tag{18}$$

After integration over Ψ and rotation to the real time it becomes finally the DOS expression

$$\int D[\zeta(x)] \delta(E[\zeta(x)] - \Omega) \exp\left[-\frac{1}{2} \int \int dx_1 dx_2 \zeta(x_1) D^{-1}(x_1 - x_2) \zeta(x_2) \right]$$

Here $E[\zeta(x)]$ is the eigenfunction in the random field ζ:

$$\frac{-\partial_x^2}{2m} \Psi + \zeta\Psi = E\Psi \,.$$

For the dispersionless phonon alone, e.g. the amplitude mode in the CDW, $D(x) = U_0(x,0) \sim \delta(x)$ and the known exact results for the uncorrelated disorder [23] provide us with the PG asymptotics

$$I(\Omega) \propto \exp\left[-\frac{8}{3^{3/2}} \frac{|W_p|}{\omega_0} \left| \frac{\Omega}{W_p} \right|^{3/2} \right] \,. \tag{19}$$

For the CDW parameters it becomes

$$I(\Omega) \propto \exp\left[-\frac{16}{3\pi}\left(2\frac{\Delta_0 - \Omega}{(\Delta_0 \omega_0^2)^{1/3}}\right)^{3/2}\right].\tag{20}$$

Below we shall concentrate only on a more problematic case of the sound mode. The correlator of the "disordered potential" ζ, $D(x)$, is just the mean square of quantum fluctuations of the phonon potential $\zeta = v_F/2\varphi'(x,t)$ at coinciding times: in the Fourier representation

$$D_k = \int \frac{d\omega}{2\pi}\frac{\lambda_s k^2}{(\omega/u)^2 + k^2} = \frac{1}{2}\lambda_s u|k|.$$

The probability distribution for the Fourier components ζ_k is

$$P[\zeta_k] \sim \exp\left(-\int \frac{dk}{2\pi}\frac{|\zeta_k|^2}{\lambda_s u|k|}\right)\tag{21}$$

which tells us that the component with $k = 0$ is excluded, $P(\zeta_0) = 0$. The constraint

$$\zeta_0 = \int_{-\infty}^{\infty} \zeta(x)dx = 0.\tag{22}$$

agrees with properties of the potential $\sim \varphi'$ in the time dependent picture of the previous section which obeys the condition (22) at any finite t, see the Fig.3. Contrary to usual expectations for the method of optimal fluctuations, here the potential well creating the level E must be accompanied by compensating barriers. The condition (22) is linked to the paradox noticed in the pervious section: an absence of a finite minimum over the length scale at a given T. Indeed, now we cannot rely upon an existence of a bound state at arbitrary shallow potential: $E_0 \sim -m\left(\int dx\zeta(x)\right)^2$ which is zero at the condition (22).

While the divergency at small k (large x) is physical, the one at large k in (21) must be regularized to work in the real space. We shall proceed by introducing the auxiliary field $\mu(x)$ such that $\zeta = d\mu/dx = \mu'$. Finally we arrive at the model of the "nonlocal acoustic disorder"

$$I(\Omega) \sim \int D[\mu(x)]\delta(E[\partial_x\mu(x)] - \Omega)\exp\left[-\frac{\lambda_s}{2u}\int\int dx_1 dx_2\frac{(\mu(x_1) - \mu(x_2))^2}{|x_1 - x_2|^2}\right]\tag{23}$$

Here the integral in the exponent is already regular at small x. The divergence at large x works to maintain the constraint (22), otherwise $\mu(+\infty) - \mu(-\infty) = \int_{-\infty}^{\infty}\zeta(x)dx \neq 0$ and the integral in (23) would diverge logarithmically leading to the zero probability.

Unfortunately we are not aware of exact studies for disordered systems with such long range correlations. Usual scaling estimations ([24]) for characteristic μ and l give us $|\Omega| \sim 1/(ml^2) \sim |\mu|/l$ then $|\mu| \sim |\Omega/m|^{1/2}$ hence $\ln I \sim -\mu^2\lambda_s/u \sim -|\Omega|\lambda_s/u$ in accordance with direct estimations and the result (17) for the generic time dependent model.

V. DISCUSSION AND CONCLUSIONS

We summarize the obtained results as follows.

The PG starts below the free edge by (stretched) exponential dependencies

$$I \sim \exp\left[-cnst\,(-|\Omega|)^{\gamma}\right] \qquad (24)$$

with different powers $\gamma = 3/2$ for gapful phonons and $\gamma = 1$ for sounds. If both modes are present, then the smallest one, with $\gamma = 3/2$, dominates at small Ω. This regime corresponds to free electronic states smeared by instantaneous uncorrelated quantum fluctuations of the lattice.

Deeply within the PG, approaching the absolute threshold W_s or W_p, the exponential law changes for the power law $I(\Omega) \propto (\Omega - W_s)^{\beta}$ with the big index β. This contribution dominates over the smooth one from gapful modes $I \sim \exp(cnst\,\delta\Omega\ln\delta\Omega)$. The power regime corresponds to creation of nearly amplitude solitons surmounted be compensating phase tails. Its description provides a quasiclassical interpretation for processes in fully quantum systems of correlated electrons in the spin-gap regime, with the AS being a version of the spinon.

These results are different from anything used earlier both in theoretical discussions and in interpretation of experimental data [13]. They can vaguely explain the unusually wide pseudogaps observed in experiments even at low temperatures for well formed ICDWs.

Our results have been derived for single electronic transitions: PES and tunneling. They can also be applied to intergap (particle-hole) optical transitions as long as semiconductors are concerned. For the ICDW results are applied to the free edge vicinity. But the edge at $2E_s$ will disappear in favor of optically active gapless phase mode.

It should be stresses in this respect that there *cannot be a common PG* for processes characterized by different time scales. We should distinguish [8] between short living states observed in optical, PES (and may be tunneling) experiments and long living states (amplitude solitons, phase solitons) contributing to the spin susceptibility, NMR relaxation, heat capacitance, conductivity, etc. States forming the optical PG are created instantaneously; particularly near the free edge they are tested over times which are shorter than the inverse phonon frequencies $\tau_{opt} \sim \hbar/E_g < \omega_{ph}^{-1}$ and many orders of magnitude beyond the life times required for current carriers, and even much longer times for thermodynamic contributions. It follows then that the analysis of different groups of experimental data within the same picture [13] must be reevaluated. The lack of discriminating different time scales concerns also typical discussions of PGs in $High - T_c$ superconductors.

We conclude that the subgap absorption in systems with gapless phonons is dominated by formation of long space-time tails of relaxation. It concerns both acoustic polarons in $1D$ semiconductors and solitons in CDWs. Near the free edge the simple exponential, Urbach type, law appears competing with stretched exponential ones typical for tails from optimal fluctuations. The deeper part of the PG is dominated by the power law singularity near the absolute edge.
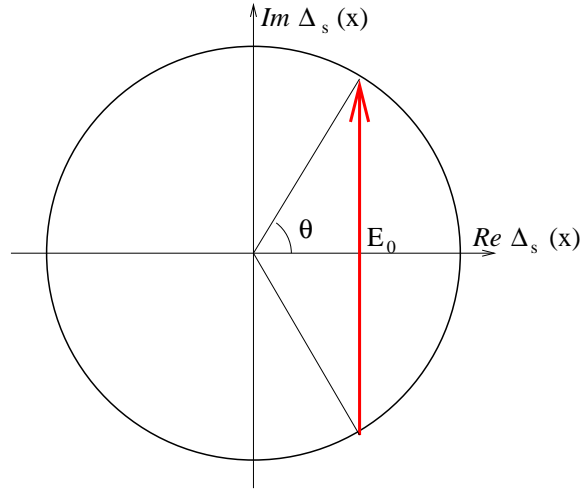
FIGURES

FIG. 1. Trajectory of the chordus soliton with phase tails in the complex plane Δ
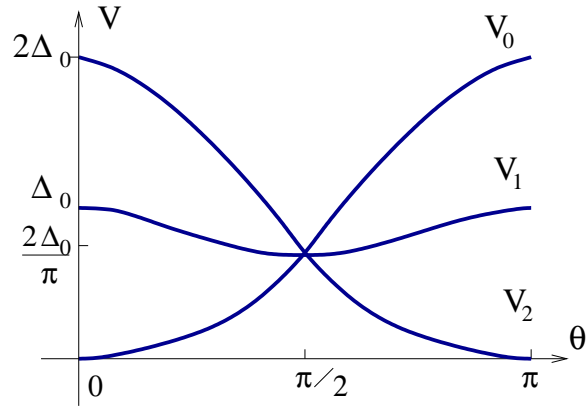

FIG. 2. Selftrapping terms V_ν for chordus solitons as functions of the chiral angle 2θ for various fillings ν.
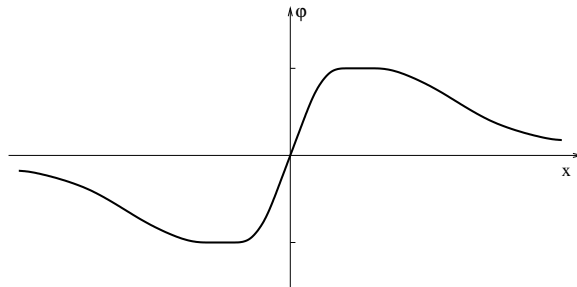

FIG. 3. The acoustic polaron field $\varphi(x,t)$ as a function of x at some moment t.

REFERENCES

[1] S. I. Matveenko and S. A. Brazovskii, Phys. Rev. B **65**, 245108 (2002).

[2] G. Grüner, Rev. Mod. Phys., **60**, 1129 (1988).

[3] P. A. Lee, T. M. Rice and P. W. Anderson, Phys. Rev. Lett. **31**, 462 (1973).

[4] S. Brazovskii and I. Dzyaloshinskii, Sov. Phys. JETP **44**, 1233 (1976).

[5] E.I. Rashba in *Excitons*, E.I. Rashba and M. D. Sturge eds., p. 543 (North-Holland, 1982).

[6] A. Bjelis and S. Barisic, J. de Physique. Lett. **36**, L169 (1975).

[7] M.V. Sadovskii, JETP **39**, 845 (1974); *ibid*, **50**, 989 (1979).

[8] S. Brazovskii, JETP Lett. **28**, 606 (1978); JETP **51**, 342 (1980).

[9] H.P. Geserich et al, Physica, **143B**, 198 (1986); L. Degiorgi et al, *Phys. Rev. B,* **49**, 14754 (1994); *ibid*, **52**, 5603 (1995).

[10] F. Nad in *Charge Density Waves in Solids*, eds. L. Gor'kov and G. Grüner, p.191 (Elsevier Sci. Publ., Amsterdam,1989).

[11] G. Minton and J.W. Brill, PRB **36**, 4254 (1987).

[12] G-H Gweon et al, J.Phys.: Cond. Matt. **8**, 9923 (1996); A. Terrasi *et al.*, Phys. Rev. B, **52**, 5592 (1995); B. *ibid*, **56**, 12647 (1997); L. Perfetti et al., Phys. Rev. Lett. **87**, 216404 (2001).

[13] R.H. McKenzie *et al.*, Phys. Rev. Let. **69**, 1085 (1992) and Phys. Rev. B **52**, 16428 (1995); K. Kim *et al.*, Phys. Rev. Let.**71**, 4015 (1993).

[14] A.S. Ioselevich, Sov. Phys. JETP **54**, 800 (1981); *ibid*, **55**, 358 (1982); *ibid* **56**, 415 (1982).

[15] A. Auerbach and S. Kivelson, Phys. Rev. **B 33**, 8171 (1986) *and refs. therein.*

[16] R. Rajaraman, *"Solitons and Instantons"*, North-Holland (1989).

[17] S.V. Iordanskii and E.I. Rashba, Sov. Phys. JETP **47**, 975 (1978).

[18] S. Brazovskii, N. Kirova in *Soviet Scientific Reviews*, Sec. A, Physics. Reviews., I. M. Khalatnikov ed., v. **5**, 99 (Harwood Acad. Publ., 1984).

[19] S. Brazovskii, "Solitons in Charge Density Waves" in *"Charge Density Waves in Solids"* Eds. L. Gor'kov and G. Grüner, Elsevier Sci. Publ., Amsterdam, 1989.

[20] S. A. Brazovskii and S. I. Matveenko, Sov. Phys. JETP **72** 492 (1991).

[21] A.O. Caldeira and A.J. Leggett, Phys. Rev. Lett. **46**, 211 (1981).

[22] S. Brazovskii, **cond-mat**/0204147 and **cond-mat**/0006355.

[23] B. Halperin, Phys. Rev. **139**, A104 (1965).

[24] I.M. Lifshits, S.A. Gredeskul and L.A. Pastur, *"Introduction to the theory of disordered systems"* (Wiley, New York, 1988).

VI. APPENDIX

Electronic energies in the complex field Δ are determined by the Dirac Hamiltonian

$$\begin{vmatrix} -iv_F\partial_x & \Delta \\ \Delta^* & iv_F\partial_x \end{vmatrix}, \quad \Delta = |\Delta|e^{i\varphi}$$

In the ground state $|\Delta(x,t)| = \Delta_0$, $\varphi = cnst$ and the electronic spectrum is $E^2 = v_F^2 k^2 + \Delta_0^2$ where v_F is the Fermi velocity. But these free states are not proper excitations. The evolution of added electrons or holes with the initial $E_0 \geq \Delta_0$ to the AS with $W_s = 2/\pi\Delta_0 < \Delta_0$ can be described by the exact solution for intermediate configurations characterized by the singly occupied arbitrary positioned intragap state $E_0 = \Delta_0 \cos\theta$ with $0 \leq \theta \leq \pi$, hence $-\Delta_0 < E_0 < \Delta_0$. It was found [8] to be the Chordus Soliton (ChS) with 2θ being the total chiral angle: $\Delta(\pm\infty) = \exp(\pm i\theta)$, see the Fig.1.

Namely,

$$\Delta_{ChS}(x,\theta) = \Delta_0(\cos\theta + i\sin\theta\tanh(k_0 x))\exp i\varphi_0, \quad k_0 = \Delta_0\sin\theta. \tag{25}$$

with an arbitrary $\varphi_0 = cnst$. The potentials V_ν are known [8] as (see Fig.2

$$V_\nu(\theta) = \Delta_0[(\nu - \frac{2}{\pi}\theta)\cos\theta + \frac{2}{\pi}\sin\theta]$$

where ν is the filling number of the intragap state that is $\nu = 0, 1$ for $j = 0, 1$ while $\nu = 2$ is equivalent to $j = 0$ for the ground state extended by the two particles $N = 2M + 2$. The term $V_0(\theta)$ increases monotonically from $V_0(0) = 0$ for the $2M$ ground state to $V_0(\pi) = 2\Delta_0$ for the $2M + 2$ ground state (GS) with two free holes. Apparently there is an opposite dependence for $V_2(\theta) = V_0(\pi - \theta)$. Thus the total phases slip $2\theta = 0 \Rightarrow 2\theta = 2\pi$ realizes the spectral flow across the gap, accompanied also by the flow of particles for $\nu = 2$ which makes it favorable. The term $V_1(\theta) = V_1(\pi - \theta)$ is symmetric describing both the particle upon the $2M$ GS and the hole upon the $2M + 2$ GS. Apparently $V_1(0) = V_1(\pi) = \Delta_0$ (the degenerate Ground States are: the $2M$ one with the additional free electron for $\theta = 0$ and the $2M + 2$ one with the additional free hole for $\theta = \pi$) while the minimum is $V_1(\pi/2) = W_s < \Delta_0$ where $W_s = 2\Delta_0/\pi$ is the AS energy. Thus the stationary state of the system with an odd number of particles, the minimum of V_1, is the amplitude soliton (AS) $\Delta \Rightarrow -\Delta$ with the midgap state $E_0 = 0$ occupied by the singe electron.

Notice that being the uncharged spin carrier with the topological charge equal unity, the AS is a quasiclassical realization of the spinon in systems with nonretarded attraction of electrons (that is with high, rather than low, phonon frequencies).